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## Selected Papers Associated with the Modeling and Design of Molecular Materials (MDMM 2022) Conference

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Deadline for manuscript  
submissions:

**closed (30 April 2023)**

### Message from the Guest Editors

Dear Colleagues,

The Modeling and Design of Molecular Materials 2022 (MDMM 2022) conference is an interdisciplinary meeting devoted to the various aspects of conceiving materials with predefined properties. The key term is “molecular material”, which in the context of the conference means drugs and drug carriers (focused on cancer), catalysts, with an emphasis on photocatalysis (e.g., solar energy conversion) or theozymes (theoretically designed biocatalysts), materials for hydrogen storage (green fuel), conductive polymers (e.g., electronics, biosensors), etc. Nowadays, computer modeling seems to be a crucial step for the rational design of materials with demanded properties. Thus, during this prospective event we hope to gather specialists who develop computational methods useful in the computer-aided design of materials as well as those who employ molecular modeling at the very early stages of their projects and for whom a computational approach eventually leads to practical solutions.



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**Special** Issue



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## Message from the Editor-in-Chief

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